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FILE COVERS 1907 - 21 Oct 2009  VOL 151 ISS 17
FILE LAST UPDATED: 20 Oct 2009  (20091020/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED:  Aug 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  Aug 2009

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d stat que l38
L3              STR
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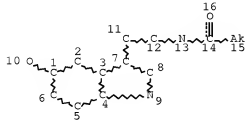


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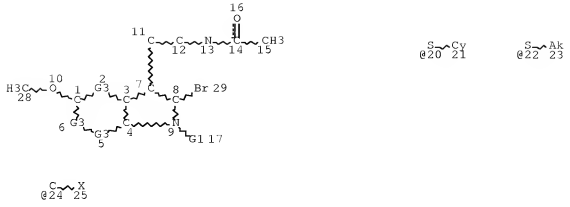

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L38 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1237889 HCAPLUS Full-text
DOCUMENT NUMBER: 149:417852
TITLE: Novel bromo-melatonin derivatives as potentially effective drugs to treat bone diseases
AUTHOR(S): Suzuki, Nobuo; Somei, Masanori; Seki, Azusa; Reiter, Russel J.; Hattori, Atsuhiko
CORPORATE SOURCE: Noto Marine Laboratory, Institute of Nature and Environmental Technology, Kanazawa University, Housu-gun, Ishikawa, Japan
SOURCE: Journal of Pineal Research (2008), 45(3), 229-234
CODEN: JPRSE9; ISSN: 0742-3098
PUBLISHER: Wiley-Blackwell
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. Several reports indicate that melatonin is involved in the regulation of bone metabolism To examine the direct effect of melatonin on osteoclasts and osteoblasts, we developed an in vitro assay using fish scales that contain osteoclasts, osteoblasts, and bone matrix, all of which are similar to those found in mammalian membrane bone. Using the assay, we demonstrated that melatonin suppressed osteoclastic and osteoblastic activities. These findings are in agreement with the reports from in vivo studies in mice and rats. In an attempt to develop mols. that increase bone mass, novel bromo-melatonin derivs. were synthesized, and the effects of these

chems. on osteoclasts and osteoblasts using the scale assay were examined As a result, novel bromo-melatonin derivs. with the ability to possibly increase bone formation were identified. In scale osteoclasts, particularly, 1-benzyl-2,4,6-tribromo-melatonin had a more potent activity than melatonin. In reference to osteoblasts, this agent (10-9-10-6 M) significantly activated osteoblasts. The effect of 1-benzyl-2,4,6-tribromo-melatonin on bone formation was confirmed in ovariectomized rats. Thus, the oral administration of 1-benzyl-2,4,6-tribromo-melatonin augmented the total bone mineral d. of the femoral metaphysis of ovariectomized rats. The stress-strain index of the diaphysis in 1-benzyl-2,4,6-tribromo-melatonin-treated rats significantly increased in comparison with that in ovariectomized rats. In rats fed a low-calcium diet, the total bone mineral d. of the femoral metaphysis significantly increased following the oral administration of 1-benzyl-2,4,6-tribromo-melatonin. These studies identified a melatonin derivative that may have potential use in the treatment of bone diseases, such as osteoporosis.

IT 864546-07-6, 1-Propargyl-2,4,6-Tribromo-melatonin
864546-08-7, 1-Allyl-2,4,6-Tribromo-melatonin
864546-09-8, 1-Benzyl-2,4,6-Tribromo-melatonin
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel bromo-melatonin derivs. as potentially effective drugs to treat bone diseases)

RN 864546-07-6 HCAPLUS
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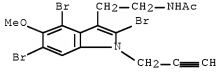

RN 864546-08-7 HCAPLUS
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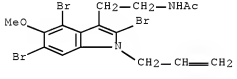
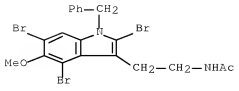


RN 864546-09-8 HCAPLUS
CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(phenylmethyl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

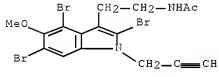
L38 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:462432 HCAPLUS Full-text
DOCUMENT NUMBER: 149:45397
TITLE: Novel bromomelatonin derivatives suppress osteoclastic activity and increase osteoblastic activity: implications for the treatment of bone diseases
AUTHOR(S): Suzuki, Nobuo; Somei, Masanori; Kitamura, Kei-Ichiro; Reiter, Russel J.; Hattori, Atsuhiko
CORPORATE SOURCE: Noto Marine Laboratory, Institute of Nature and Environmental Technology, Kanazawa University, Housu-gun, Ishikawa, Japan
SOURCE: Journal of Pineal Research (2008), 44(3), 326-334
CODEN: JPRSE9; ISSN: 0742-3098
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The teleost scale is a calcified tissue that contains osteoclasts, osteoblasts, and bone matrix, all of which are similar to those found in mammalian membrane bone. Using the goldfish scale, we recently developed a new in vitro assay system and previously demonstrated that melatonin suppressed both osteoclastic and osteoblastic activities in this assay system. In mammals, 2-bromomelatonin possesses a higher affinity for the melatonin receptor than does melatonin. Using a newly developed synthetic method, we synthesized 2-bromomelatonin, 2,4,6-tribromomelatonin and novel bromomelatonin derivs. (1-allyl-2,4,6-tribromomelatonin, 1-propargyl-2,4,6-tribromomelatonin, 1-benzyl-2,4,6-tribromomelatonin, and 2,4,6,7-tetrabromomelatonin) and then examined the effects of these chems. on osteoclasts and osteoblasts. All bromomelatonin derivs., as well as melatonin, had an inhibitory action on osteoclasts. In particular, 1-benzyl-2,4,6-tribromomelatonin (benzyl-tribromomelatonin) possessed a stronger activity than melatonin. At an in vitro concentration of 10-10 M, benzyl-tribromomelatonin still suppressed osteoclastic activity after 6 h of incubation. In reference to osteoblasts, all bromomelatonin derivs. had a stimulatory action, although melatonin inhibited osteoblastic activity. In addition, estrogen receptor mRNA expression (an osteoblastic marker) was increased in benzyl-tribromomelatonin (10-7 M)-treated scales. Taken together, the present results strongly suggest that these novel melatonin derivs. have significant potential for use as beneficial drug for bone diseases such as osteoporosis.

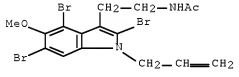
IT 864546-07-6P, 1-Propargyl-2,4,6-tribromomelatonin
864546-08-7P, 1-Allyl-2,4,6-tribromomelatonin
864546-09-8P, 1-Benzyl-2,4,6-tribromomelatonin
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(novel bromomelatonin derivs. suppress osteoclastic activity and increase osteoblastic activity: implications for treatment of bone diseases)

RN 864546-07-6 HCAPLUS
CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(2-propyn-1-yl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 864546-08-7 HCAPLUS
CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(2-propen-1-yl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 864546-09-8 HCAPLUS
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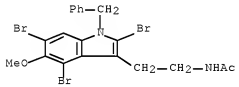

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:82570 HCAPLUS Full-text
DOCUMENT NUMBER: 146:163392
TITLE: Preparation of tryptophan derivatives for the treatment of osteoporosis
INVENTOR(S): Somei, Masanori; Hattori, Atsuhiko; Suzuki, Nobuo
PATENT ASSIGNEE(S): National University Corporation Kanazawa University, Japan; National University Corporation Tokyo Medical

and Dental University
SOURCE: PCT Int. Appl., 28pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 20070107 23	A1	20070125	WO 2006-JP312978	20060629
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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1911744	A1	20080416	EP 2006-767595	20060629
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
US 20090054511	A1	20090226	US 2008-7992	20080117
CN 101233105	A	20080730	CN 2006-80026616	20080121
PRIORITY APPLN. INFO.:			JP 2005-209753 A	20050720
			WO 2006-JP312978 W	20060629

OTHER SOURCE(S): MARPAT 146:163392
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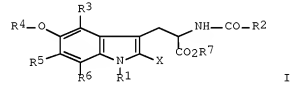

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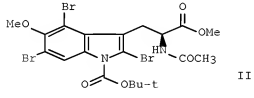


II

AB Title compds. I [X = halo; R1 = H, (un)substituted alkyl, (un)substituted alkenyl, etc.; R2 = (un)substituted alkyl; R3, R5, R6 = H, halo; R4 = H, (un)substituted alkyl; R7 = H, (un)substituted hydrocarbon group] and salts

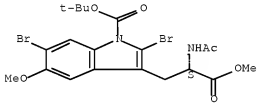
thereof were prepared For example, reaction of (S)-N-acetyl-2,4,6-tribromo-5-methoxytryptophan Me ester, e.g., prepared from (S)-N-acetyl-5-methoxytrytophan Me ester, with BOC2O afforded compound II. The disclosed tryptophan derivs. were tested for the influences by tartarate resistant acid phosphatase (TRAP) and alkali phosphatase (ALP), and showed inhibition of osteoclast and activation of osteoblast.

IT 920516-24-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of tryptophan derivs. for the treatment of osteoporosis)

RN 920516-24-1 HCAPLUS

CN L-Tryptophan, N-acetyl-2,6-dibromo-1-[(1,1-dimethylethoxy)carbonyl]-5-methoxy-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

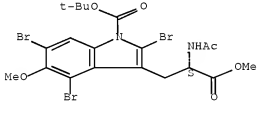


IT 920516-20-7P 920516-21-8P 920516-22-9P
920516-23-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tryptophan derivs. for the treatment of osteoporosis)

RN 920516-20-7 HCAPLUS

CN L-Tryptophan, N-acetyl-2,4,6-tribromo-1-[(1,1-dimethylethoxy)carbonyl]-5-methoxy-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 920516-21-8 HCAPLUS

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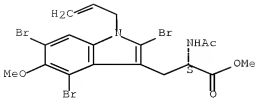
Absolute stereochemistry. Rotation (+).



RN 920516-22-9 HCAPLUS
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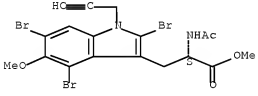
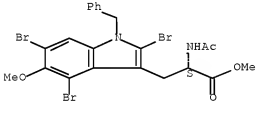
Absolute stereochemistry. Rotation (+).



RN 920516-23-0 HCAPLUS
CN L-Tryptophan, N-acetyl-2,4,6-tribromo-5-methoxy-1-(phenylmethyl)-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:	2006:319103 HCAPLUS Full-text
DOCUMENT NUMBER:	144:343589
TITLE:	α2 RECEPTOR BLOCKING AGENT CONTAINING INDOLE DERIVATIVE AS ACTIVE INGREDIENT AND VASODILATOR
INVENTOR(S):	Somei, Masanori; Shigenobu, Koki; Tanaka, Yoshio
PATENT ASSIGNEE(S):	National University Corporation Kanazawa University, Japan; The Toho University
SOURCE:	PCT Int. Appl., 22 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	Japanese
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006035617	A1	20060406	WO 2005-JP17109	20050916
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
JP 2006089443	A	20060406	JP 2004-280104	20040927
JP 3964417	B2	20070822		
US 20090005430	A1	20090101	US 2007-663748	20070823
PRIORITY APPLN. INFO.:			JP 2004-280104 A	20040927
			WO 2005-JP17109 W	20050916

OTHER SOURCE(S): MARPAT 144:343589

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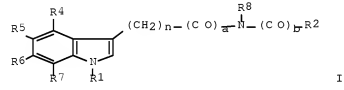


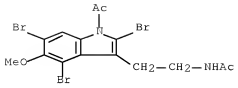
I

AB A compound having a simpler structure than yohimbine, which is a pentacyclic fused heterocyclic compound, and having an activity similar to that of yohimbine. Also provided is an α2 receptor blocking medicine or food composition containing either a compound represented by the formula : [Chemical formula I] (wherein R1 represents hydrogen, alkyl, alkenyl, alkynyl, an aromatic group, aralkyl, acyl, arylsulfonyl, alkylsulfonyl, or hydroxy; R2 represents a hydrocarbon group; R3, R4, R5, R6, and R7 are the same or different and each represents hydrogen, halogeno, alkyl, or alkoxy; R8 represents hydrogen or acyl; n is an integer of 1-6; and a and b are the same or different and each is 1 or 0) or a pharmaceutically acceptable salt thereof.

IT 300662-22-0, 1-Acetyl-2,4,6-tribromomelatonin
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(indole and melatonin derivs. as α2-adrenergic receptor antagonists and vasodilators)

RN 300662-22-0 HCAPLUS

CN Acetamide, N-[2-(1-acetyl-2,4,6-tribromo-5-methoxy-1H-indol-3-yl)ethyl]- (CA INDEX NAME)

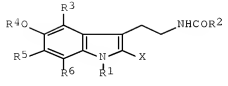


OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1004558 HCAPLUS Full-text
DOCUMENT NUMBER: 143:306168
TITLE: Preparation of indole derivatives for treatment of osteoporosis
INVENTOR(S): Somei, Masanori; Hattori, Atsuhiko; Suzuki, Nobuo
PATENT ASSIGNEE(S): Kanazawa University Technology Licensing Organization Ltd., Japan
SOURCE: PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005084664	A1	20050915	WO 2005-JP3743	20050304
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2005289985	A	20051020	JP 2005-61080	20050304
JP 4014052	B2	20071128		
US 20070197629	A1	20070823	US 2006-591899	20060907
PRIORITY APPLN. INFO.:			JP 2004-64408 A	20040308
			WO 2005-JP3743 W	20050304

OTHER SOURCE(S): MARPAT 143:306168
GI

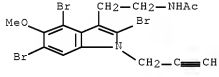


I

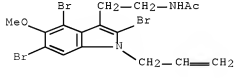
AB Title compds. represented by the formula I [wherein X = halo; R1 = H, (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = (un)substituted alkyl; R3, R5, R6 = independently H or halo; R4 = H or (un)substituted alkyl; and pharmaceutically acceptable salts thereof] were prepared for treatment of osteoporosis. For example, reaction of I (X = R3 = R5 = Br, R2 = R4 = Me, R1 = H) with propargyl chloride gave I (R2-R6 are defined as above, R1 = CH.tplbond.CCH2) in 97% yield. The indole derivs. were tested for the influences received by bone cell (TRAP activity) and osteoblastic cell (ALP activity), and showed inhibition of osteoclast and activation of osteoblastic cell. Thus, I and their pharmaceutical compns. are useful for the treatment of osteoporosis.

IT 864546-07-6P 864546-08-7P 864546-09-8P
864546-10-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indole derivs. for treatment of osteoporosis)

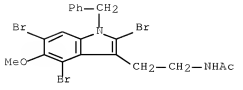
RN 864546-07-6 HCAPLUS
CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(2-propyn-1-yl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



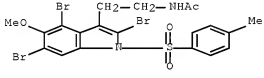
RN 864546-08-7 HCAPLUS
CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(2-propen-1-yl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 864546-09-8 HCAPLUS
CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(phenylmethyl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)

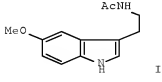


RN 864546-10-1 HCAPLUS
CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-[(4-methylphenyl)sulfonyl]-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



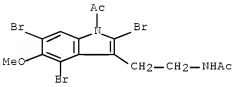
OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:557901 HCAPLUS Full-text
DOCUMENT NUMBER: 133:296316
TITLE: Syntheses of melatonin and its derivatives
AUTHOR(S): Somei, Masanori; Fukui, Yoshikazu; Hasegawa, Masakazu; Oshikiri, Naoki; Hayashi, Toshikatsu
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Kanazawa University, Kanazawa, 920-0934, Japan
SOURCE: Heterocycles (2000), 53(8), 1725-1736
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:296316
GI



AB Two simple synthetic methods for melatonin (I) are newly developed from tryptamine through intermediates, which are promising lead compds. for drug developing research. Novel chemical reactivities of melatonin in its bromination, lithiation, and acylation are also reported.

IT 300662-22-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of melatonin and derivs.)
RN 300662-22-0 HCAPLUS
CN Acetamide, N-[2-(1-acetyl-2,4,6-tribromo-5-methoxy-1H-indol-3-yl)ethyl]-
(CA INDEX NAME)



OS.CITING REF COUNT: 22 THERE ARE 22 CAPLUS RECORDS THAT CITE THIS RECORD (23 CITINGS)
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:996976 HCAPLUS Full-text
DOCUMENT NUMBER: 124:175864
ORIGINAL REFERENCE NO.: 124:32611a,32614a
TITLE: Preparation of spiro[indole-3,3'-pyrrolidine] derivatives as melatoninergic agonists
INVENTOR(S): Fourtillan, Jean-Bernard; Fourtillan, Marianne; Jacquesy, Jean-Claude; Jouannetaud, Marie-Paule; Violeau, Bruno; Karam, Omar
PATENT ASSIGNEE(S): CEMAF, Fr.
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9527712	A1	19951019	WO 1995-FR443	19950406
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
FR 2718445	A1	19951013	FR 1994-4102	19940407
FR 2718445	B1	19960628		
FR 2724170	A1	19960308	FR 1994-10558	19940902
FR 2724170	B1	19970530		
AU 9523108	A	19951030	AU 1995-23108	19950406
EP 754183	A1	19970122	EP 1995-916720	19950406
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1148855	A	19970430	CN 1995-192961	19950406
CN 1047386	C	19991215		
JP 09511514	T	19971118	JP 1995-526122	19950406
ZA 9509826	A	19960529	ZA 1995-9826	19951120

US 5763471	A	19980609	US 1996-722105		19961211
PRIORITY APPLN. INFO.:			FR 1994-4102	A	19940407
			FR 1994-10558	A	19940902
			WO 1995-FR443	W	19950406

OTHER SOURCE(S): CASREACT 124:175864; MARPAT 124:175864

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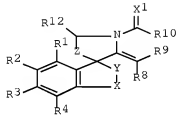

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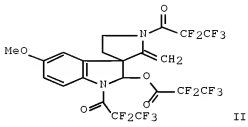


II

AB Title compds. [I; R1-R4 = H, halo, alkyl, alkoxy, etc.; R8,R9 = H, alkyl, aryl(alkyl); R10 = H, alkyl, aryl, etc.; R12 = H, alkyl; XY = NR5CR6R7, NR5C(:X3), N:CR14; R5 = H, alkyl, aryl, etc.; R6,R7 = H, alkyl, aryl, etc.; R14 = H, alkyl, alkoxy, etc.; X1,X3 = O, S, (alkyl)imino; Z = CH2, CH2CH2] were prepared Thus, melatonin was treated with pentafluoropropionic anhydride to give title compound II. Data for sedative-hypnotic activity of I in vivo were given.

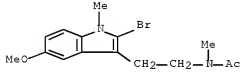
IT 173589-57-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of spiro[indole-3,3'-pyrrolidine] derivs. as melatoninergic agonists)

RN 173589-57-6 HCAPLUS

CN Acetamide, N-[2-(2-bromo-5-methoxy-1-methyl-1H-indol-3-yl)ethyl]-N-methyl- (CA INDEX NAME)



OS.CITING REF COUNT:	5	THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT:	6	THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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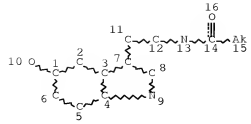

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE
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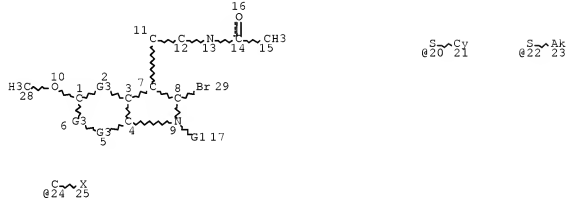
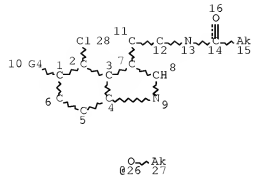
L15 STR



VAR G1=AK/CY/20/22
VAR G3=CH/24
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
L16 19 SEA FILE=REGISTRY SUB=L5 SSS FUL L15
L23 STR



VAR G4=OH/26
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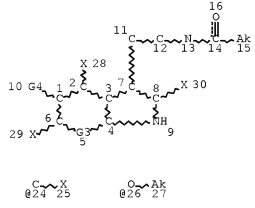
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L25 STR



VAR G3=CH/24
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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE
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L38 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L16
L39 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L27
L40 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L39 NOT L38

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L40  ANSWER 1 OF 3  HCAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         1993:254747  HCAPLUS  Full-text
DOCUMENT NUMBER:          118:254747
ORIGINAL REFERENCE NO.:   118:44261a,44264a
TITLE:                    Tryptamine analogues, their synthesis and their use as
                          5-HT1-like or 5-HT2 receptor agonists
INVENTOR(S):              Kruse, Lawrence Ivan; Young, Rodney Christopher;
                          Kaumann, Alberto Julio
PATENT ASSIGNEE(S):       SmithKline Beecham PLC, UK
SOURCE:                   PCT Int. Appl., 45 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
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     WO 9300333           A1    19930107    WO 1992-GB1089         19920617
         W:  AU, CA, JP, KR, US
         RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE
     AU 9219288           A     19930125    AU 1992-19288          19920617
     EP 593513            A1    19940427    EP 1992-912269         19920617
     EP 593513            B1    19981028
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE
     JP 06508354          T     19940922    JP 1992-511317         19920617
     AT 172723            T     19981115    AT 1992-912269         19920617
     ZA 9204523           A     19931220    ZA 1992-4523           19920619
     CA 2110574           A1    19930107    CA 1992-2110574        19920717
     US 5571833           A     19961105    US 1994-167890         19940526
PRIORITY APPLN. INFO.:                       GB 1991-13382      A   19910621
                                             GB 1991-13385      A   19910621
                                             WO 1992-GB1089     A   19920617
OTHER SOURCE(S):          MARPAT 118:254747
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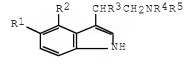
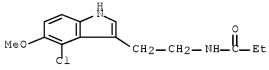


I

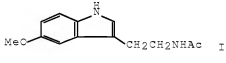
AB Title compds. I (R1 = H, HO, C1-4 alkoxy, halo-C1-4-alkoxy, C3-7-cycloalkyl-C1-4-alkoxy, aryloxy, aryl-C1-4-alkoxy; R2 = halo, C1-4 alkyl, NC, O2N, F3C; R3 = H, C1-4 alkyl; R4, R5 = H, C1-4 alkyl, R4R5N = ring), were prepared Thus, 3-(cyanomethyl)-4-chloro-5-(benzyloxy)indole (preparation given) in MeOH/NH3 was hydrogenated over Raney Ni to give I (R1 = PhCH2O, R2 = Cl, R3 = H, R4 = R5 Me) which was hydrogenated over Pd-C and treated with (CO2H)2 to give I (R1 = HO, R2 = Cl, R3 = H, R4 = R5 = Me) oxalate (II). In test for 5-HT1-like and 5-HT2 receptor screens, the EC50 of II was 0.2-15 and 0.2 μM, resp. Pharmaceutical formulations containing I are given.

IT 147405-70-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of serotoninergic agonists)
RN 147405-70-7 HCAPLUS
CN Propanamide, N-[2-(4-chloro-5-methoxy-1H-indol-3-yl)ethyl]- (CA INDEX NAME)



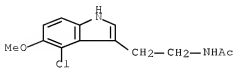
OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1981:41707 HCAPLUS Full-text
DOCUMENT NUMBER: 94:41707
ORIGINAL REFERENCE NO.: 94:6713a,6716a
TITLE: Structure-activity relationship of melatonin analogs
AUTHOR(S): Frohn, M. A.; Seaborn, C. J.; Johnson, D. W.; Phillipou, G.; Seamark, R. F.; Matthews, C. D.
CORPORATE SOURCE: Dep. Obstet. Gynaecol., Queen Elizabeth Hosp., Woodville, 5011, Australia
SOURCE: Life Sciences (1980), 27(22), 2043-6
CODEN: LIFSAK; ISSN: 0024-3205
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



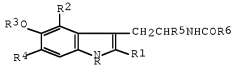
AB Anal. of the structure-activity relation between 23 indoleamines and melatonin (I) [73-31-4] based on a specific in vivo fish bioassay, is described. The results clearly define that only halogenation at position 6 or extension of the acetyl side-chain to propionyl or butyryl is tolerated without a decrease in activity. Removal of the indole double bond however, only leads to <10-fold loss of activity. The over-all relevance of the data in the development of a metabolically stable I agonist is discussed.
IT 68935-44-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(biol. activity of, structure in relation to)
RN 68935-44-4 HCAPLUS

CN Acetamide, N-[2-(4-chloro-5-methoxy-1H-indol-3-yl)ethyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L40 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1979:48848 HCAPLUS Full-text
DOCUMENT NUMBER: 90:48848
ORIGINAL REFERENCE NO.: 90:7741a,7744a
TITLE: Synthesis and evaluation of the antiovulatory activity of a variety of melatonin analogs
AUTHOR(S): Flaugh, Michael E.; Crowell, Thomas A.; Clemens, James A.; Sawyer, Barry D.
CORPORATE SOURCE: Lilly Res. Lab., Eli Lilly and Co., Indianapolis, IN, USA
SOURCE: Journal of Medicinal Chemistry (1979), 22(1), 63-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



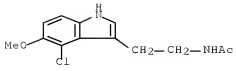
I

AB The synthesis and ovulation-inhibiting activity in rats of 14 melatonin [73-31-4] analogs I (R and R1 = H or Me; R2 = H or Cl; R3 = H, Me, Et, or Pr; R4 = H, Me, Cl, or F; R5 = H or Me; R6 = Me, Et, Pr, or adamantyl) is described. The halogenated derivs. I (R = R1 = R2 = R5 = H, R3 = R6 = Me, R4 = Cl) [63762-74-3] and I (R = R1 = R2 = R5 = H, R3 = R6 = Me, R4 = F) [62106-00-7] displayed a pronounced enhancement of ovulation-inhibiting activity. Structure-activity relations are discussed.

IT 68935-44-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and ovulation inhibiting activity of)

RN 68935-44-4 HCAPLUS

CN Acetamide, N-[2-(4-chloro-5-methoxy-1H-indol-3-yl)ethyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 21 THERE ARE 21 CAPLUS RECORDS THAT CITE THIS RECORD (21 CITINGS)

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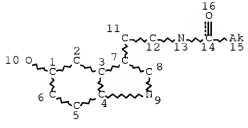
L3 STR



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NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE
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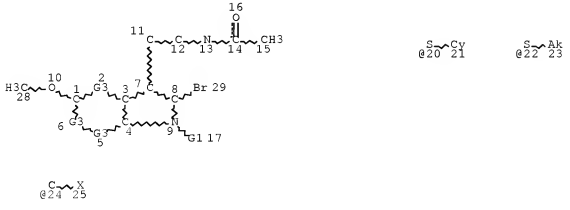

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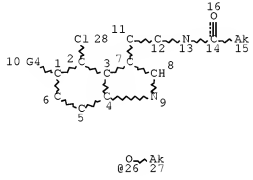
L23 STR



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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
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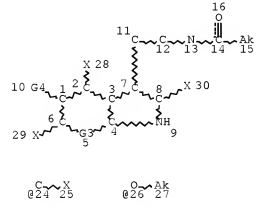

VAR G3=CH/24
VAR G4=OH/26
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE
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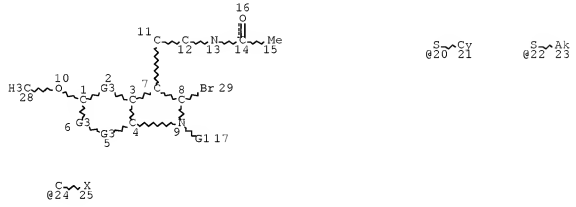
L28 STR



VAR G1=AK/CY/20/22
VAR G3=CH/24
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
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L38 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L16
L39 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L27
L40 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L39 NOT L38
L41 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L29
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=> => d stat que 144
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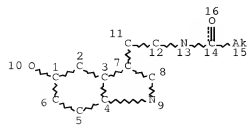

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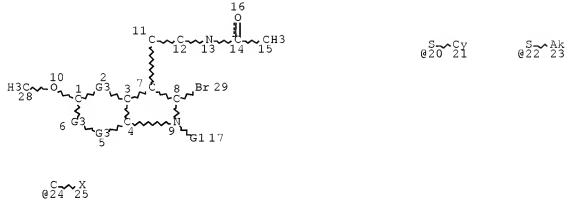
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE
L5 2378 SEA FILE=REGISTRY SSS FUL L3
L15 STR



VAR G1=AK/CY/20/22
VAR G3=CH/24
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
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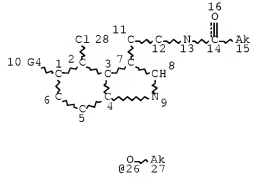
L23 STR



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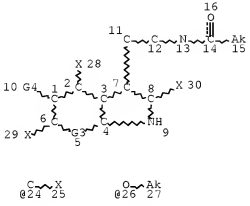
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L25 STR



VAR G3=CH/24
VAR G4=OH/26
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE
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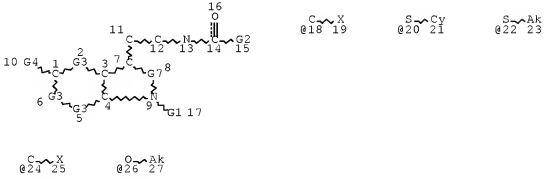
L34 STR



VAR G1=AK/CY/20/22/OH
VAR G2=AK/CY
VAR G3=CH/24
VAR G4=OH/26
VAR G7=CH/18
NODE ATTRIBUTES:

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  27

STEREO ATTRIBUTES: NONE
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L36              STR
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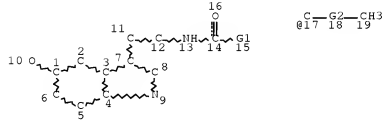

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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  19

STEREO ATTRIBUTES: NONE
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L39            9 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L27
L40            3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L39 NOT L38
L43            9 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L37
L44            9 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L43 NOT (L38 OR L40)


=> d ibib abs hitstr l44 1-9

L44  ANSWER 1 OF 9  HCAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         2008:505155  HCAPLUS  Full-text
DOCUMENT NUMBER:          148:495788
TITLE:                    Preparation of indole derivatives, especially
                          N-[β-substituted
                          (5-heterocyclylalkyloxy-1H-indol-3-yl)ethyl]amides, as
                          melatonin receptors ligands and their pharmaceutical
                          compositions
INVENTOR(S):              Marchand, Pascal; Babonneau, Vincent; Piessard,
                          Sylvie; Duflos, Sylvie; Boutin, Jean Albert; Audinot,
                          Valerie; Delagrange, Philippe; Caignard, Daniel Henri
PATENT ASSIGNEE(S):       Les Laboratoires Servier, Fr.
SOURCE:                   Fr. Demande, 22 pp.
                          CODEN: FRXXBL
DOCUMENT TYPE:            Patent
LANGUAGE:                 French
```

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

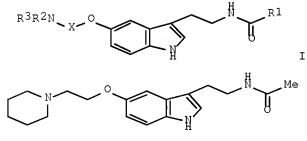
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2907451	A1	20080425	FR 2006-9113	20061018
FR 2907451	B1	20081212		
AU 2007310770	A1	20080502	AU 2007-310770	20071017
CA 2666522	A1	20080502	CA 2007-2666522	20071017
WO 2008049997	A2	20080502	WO 2007-FR1708	20071017
WO 2008049997	A3	20080912		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

EP 2079689	A2	20090722	EP 2007-858468	20071017
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS				
KR 2009084874	A	20090805	KR 2009-710133	20071017
CN 101522616	A	20090902	CN 2007-80037231	20090403
MX 2009004006	A	20090428	MX 2009-4006	20090416
NO 2009001779	A	20090506	NO 2009-1779	20090506
PRIORITY APPLN. INFO.:			FR 2006-9113 A	20061018
			WO 2007-FR1708 W	20071017

OTHER SOURCE(S): CASREACT 148:495788; MARPAT 148:495788
GI

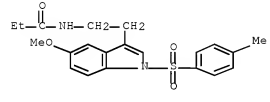


AB Title compds. I [R1 = linear or branched alkyl, cycloalkyl, cycloalkylalkyl; NR2R3 = 5-8 membered heterocycle ring; X = (CH2)n; n = 2-6; and their enantiomers and diastereomers, and their and pharmaceutically acceptable acid or base addition salts] were prepared as melatonin receptors ligands. Five biol. tests are given. Thus, condensation of nitromethane with 5-methoxy-1H-indole-3-carboxaldehyde, reduction of 5-methoxy-3-(2-nitroethenyl)-1H-indole, acylation of the amine with acetic anhydride, treatment with p-tosyl chloride, demethylation of N-[2-[5-methoxy-1-[(4-methylphenyl)sulfonyl]-1H-indol-3-

yl]ethyl]acetamide, O-alkylation of hydroxyindole with 1-(2-chloroethyl)piperidine hydrochloride, and removal of the tosyl group gave indole II. I displayed Ki values of < 1 μM for the binding to MT1 and MT2 melatonin receptors in an assay using 2-[125I]-iodomelatonin as radioligand. I acted powerfully on the circadian rhythm via melatoninergic system (no data). I are useful for treating melatoninergic system related diseases.

IT 1020701-57-8P, N-[2-[5-Methoxy-1-[(4-methylphenyl)sulfonyl]-1H-indol-3-yl]ethyl]propanamide 1020701-58-9P, N-[2-[5-Hydroxy-1-[(4-methylphenyl)sulfonyl]-1H-indol-3-yl]ethyl]propanamide 1020701-59-0P, N-[2-[1-[(4-Methylphenyl)sulfonyl]-5-[2-(1-piperidinyl)ethoxy]-1H-indol-3-yl]ethyl]propanamide 1020701-60-3P, N-[2-[5-Methoxy-1-[(4-methylphenyl)sulfonyl]-1H-indol-3-yl]ethyl]butanamide 1020701-61-4P, N-[2-[5-Hydroxy-1-[(4-methylphenyl)sulfonyl]-1H-indol-3-yl]ethyl]butanamide 1020701-62-5P, N-[2-[1-[(4-Methylphenyl)sulfonyl]-5-[2-(1-piperidinyl)ethoxy]-1H-indol-3-yl]ethyl]butanamide 1020701-63-6P
RL: PRPH (Prophetic); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-[β-substituted (5-heterocyclylalkyloxy-1H-indol-3-yl)ethyl]amides as melatonin receptor ligands)

RN 1020701-57-8 HCAPLUS
CN Propanamide, N-[2-[5-methoxy-1-[(4-methylphenyl)sulfonyl]-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 1020701-58-9 HCAPLUS
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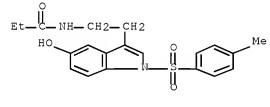

RN 1020701-59-0 HCAPLUS
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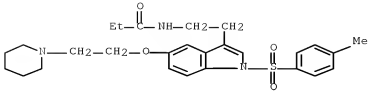

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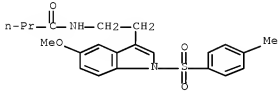
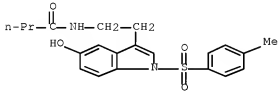


RN 1020701-61-4 HCAPLUS
CN Butanamide, N-[2-[5-hydroxy-1-[(4-methylphenyl)sulfonyl]-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 1020701-62-5 HCAPLUS
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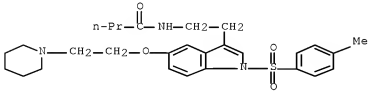

RN 1020701-63-6 HCAPLUS
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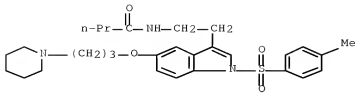


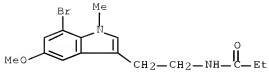
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:590020 HCAPLUS Full-text
DOCUMENT NUMBER: 147:181675
TITLE: 7-Substituted-melatonin and 7-substituted-1-methylmelatonin analogues: Effect of substituents on potency and binding affinity
AUTHOR(S): Faust, Ruediger; Garratt, Peter J.; Trujillo Perez, Maria Angeles; Piccio, Vincent J.-D.; Madsen, Christian; Stenstrom, Ane; Frolund, Bente; Davidson, Kathryn; Teh, Muy-Teck; Sugden, David
CORPORATE SOURCE: Department of Chemistry, University College London, London, WC1H 0AJ, UK
SOURCE: Bioorganic & Medicinal Chemistry (2007), 15(13), 4543-4551
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:181675

AB A series of 7-substituted melatonin and 1-methylmelatonin analogs were prepared and tested against human and amphibian melatonin receptors. 7-Substituents reduced the agonist potency of all the analogs in the Xenopus laevis melanophore assay, 7-bromomelatonin (5d) and N-Butanoyl 7-bromo-5-methoxytryptamine (5f) being the most active compds., but both were 42-fold less potent than melatonin (1). Whereas all the analogs bind with lower affinity at the human MT1 receptor than melatonin, 5d, 5f and N-Propanoyl 7-bromo-5-methoxytryptamine (5e) show a similar binding affinity to melatonin at the MT2 receptor and consequently show some MT2 selectivity. These results suggest that the receptor pocket around C-7 favors binding by an electroneg. group, suggesting an electropos. region in this area of the receptor.

IT 944478-06-2P 944478-07-3P
RL: BSU (Biological study, unclassified); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(effects of 7-Substituted-melatonin and 7-substituted-1-methylmelatonin analogs on potency and binding affinity)

RN 944478-06-2 HCAPLUS
CN Propanamide, N-[2-(7-bromo-5-methoxy-1-methyl-1H-indol-3-yl)ethyl]- (CA INDEX NAME)



RN 944478-07-3 HCAPLUS
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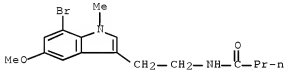


OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

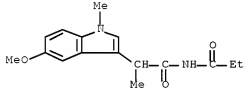
L44 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:429473 HCAPLUS Full-text
DOCUMENT NUMBER: 145:116689
TITLE: Mapping the Melatonin Receptor. 7. Subtype Selective Ligands Based on β-Substituted N-Acyl-5-methoxytryptamines and β-Substituted N-Acyl-5-methoxy-1-methyltryptamines
AUTHOR(S): Tsotinis, Andrew; Vlachou, Margarita; Papahatjis, Demetris P.; Calogeropoulou, Theodora; Nikas, Spyros P.; Garratt, Peter J.; Piccio, Vincent; Vonhoff, Stefan; Davidson, Kathryn; Teh, Muy-Teck; Sugden, David
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Athens, Athens, 157 71, Greece
SOURCE: Journal of Medicinal Chemistry (2006), 49(12), 3509-3519
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:116689

AB A series of β-substituted and β,β-disubstituted N-acyl 5-methoxy-1-methyltryptamines and 5-methoxytryptamines have been prepared as melatonin analogs to investigate the nature of the binding site of the melatonin receptor. The affinity of analogs was determined in a radioligand binding assay using cloned human MT1 and MT2 receptor subtypes expressed in NIH 3T3 cells. Agonist and antagonist potency of all analogs was measured using the pigment aggregation response of a clonal line of Xenopus laevis melanophores. β-Methylmelatonin (17a) and β,β-dimethylmelatonin (17b), though showing a slight decrease in binding at human receptors, show an increase in potency on Xenopus. N-Butanoyl 5-methoxy-1-methyl-β,β-trimethylenetryptamine (12c) is an

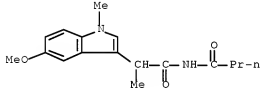
antagonist at human MT1 receptors but an agonist at MT2, while N-butanoyl 5-methoxy-1-methyl-β,β-tetramethylenetryptamine (13c) is an antagonist at MT1 but had no action at MT2 and is one of the first examples of an MT1 selective antagonist.

IT 896101-55-6P 896101-56-7P 896101-58-9P
896101-59-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Mapping the Melatonin Receptor. 7. Subtype Selective Ligands Based on β-Substituted N-Acyl-5-methoxytryptamines and β-Substituted)

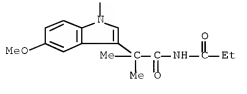
RN 896101-55-6 HCAPLUS
CN 1H-Indole-3-acetamide, 5-methoxy-α,1-dimethyl-N-(1-oxopropyl)- (CA INDEX NAME)



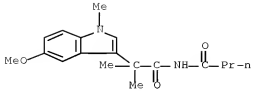
RN 896101-56-7 HCAPLUS
CN 1H-Indole-3-acetamide, 5-methoxy-α,1-dimethyl-N-(1-oxobutyl)- (CA INDEX NAME)



RN 896101-58-9 HCAPLUS
CN 1H-Indole-3-acetamide, 5-methoxy-α,α,1-trimethyl-N-(1-oxopropyl)- (CA INDEX NAME)



RN 896101-59-0 HCAPLUS
CN 1H-Indole-3-acetamide, 5-methoxy-α,α,1-trimethyl-N-(1-oxobutyl)- (CA INDEX NAME)



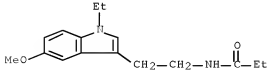
OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:347137 HCAPLUS Full-text
DOCUMENT NUMBER: 144:460948
TITLE: Structure-activity relationships of antioxidant activity of some melatonin derivatives
AUTHOR(S): Ates Alagoz, Zeynep
CORPORATE SOURCE: Eczacilik Fakultesi, Farmasotik Kimya Anabilim Dali, Ankara Universitesi, Tandogan - Ankara, 06100, Turk.
SOURCE: Ankara Universitesi Eczacilik Fakultesi Dergisi (2005), 34(2), 73-93
CODEN: AUEDE5; ISSN: 1015-3918
PUBLISHER: Ankara Universitesi Eczacilik Fakultesi
DOCUMENT TYPE: Journal
LANGUAGE: Turkish

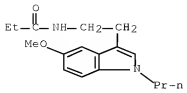
AB In the present study, thermodn., hydrophobic and steric parameters of melatonin and 23 derivs. were calculated to explain their physicochem. properties, and these parameters were compared with their antioxidant activity. Statistics methods, mainly regression anal., were used in the structure-activity relationship studies.

IT 867364-62-3 867364-63-4 867364-64-5
867364-65-6 867364-66-7
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antioxidant activity and physiochem. properties in relation to structures of melatonin derivs.)

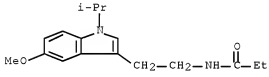
RN 867364-62-3 HCAPLUS
CN Propanamide, N-[2-(1-ethyl-5-methoxy-1H-indol-3-yl)ethyl]- (CA INDEX NAME)



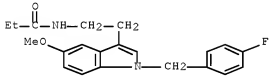
RN 867364-63-4 HCAPLUS
CN Propanamide, N-[2-(5-methoxy-1-propyl-1H-indol-3-yl)ethyl]- (CA INDEX NAME)



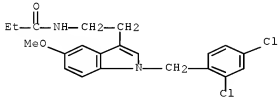
RN 867364-64-5 HCAPLUS
CN Propanamide, N-[2-[5-methoxy-1-(1-methylethyl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 867364-65-6 HCAPLUS
CN Propanamide, N-[2-[1-[(4-fluorophenyl)methyl]-5-methoxy-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 867364-66-7 HCAPLUS
CN Propanamide, N-[2-[1-[(2,4-dichlorophenyl)methyl]-5-methoxy-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



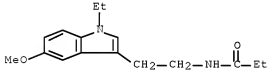
L44 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1024520 HCAPLUS Full-text
DOCUMENT NUMBER: 143:399969
TITLE: Synthesis and antioxidant properties of some indole ethylamine derivatives as melatonin analogs

AUTHOR(S): Ates-Alagoz, Z.; Buyukbingol, Z.; Buyukbingol, E.
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Department of Biochemistry2, Faculty of Pharmacy (ECZACILIK), University of Ankara, Tandogan, Ankara, 06100, Turk.
SOURCE: Pharmazie (2005), 60(9), 643-647
CODEN: PHARAT; ISSN: 0031-7144
PUBLISHER: Govi-Verlag Pharmazeutischer Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:399969

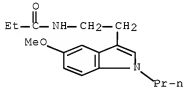
AB The synthesis and lipid peroxidn. (LP) inhibition activity of several novel indole melatonin analogs are reported. Compds. have shown variable antioxidant features depending on the substitution pattern. Melatonin and the antioxidant reference compound Bu hydroxy toluen (BHT) were used to compare the antioxidant capability of the compds. synthesized.

IT 867364-62-3P 867364-63-4P 867364-64-5P
867364-65-6P 867364-66-7P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and antioxidant properties of some indole ethylamine derivs. as melatonin analogs)

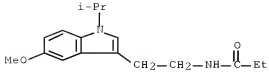
RN 867364-62-3 HCAPLUS
CN Propanamide, N-[2-(1-ethyl-5-methoxy-1H-indol-3-yl)ethyl]- (CA INDEX NAME)



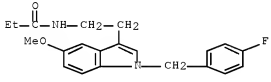
RN 867364-63-4 HCAPLUS
CN Propanamide, N-[2-(5-methoxy-1-propyl-1H-indol-3-yl)ethyl]- (CA INDEX NAME)



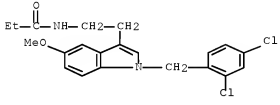
RN 867364-64-5 HCAPLUS
CN Propanamide, N-[2-[5-methoxy-1-(1-methylethyl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 867364-65-6 HCAPLUS
CN Propanamide, N-[2-[1-[(4-fluorophenyl)methyl]-5-methoxy-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 867364-66-7 HCAPLUS
CN Propanamide, N-[2-[1-[(2,4-dichlorophenyl)methyl]-5-methoxy-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

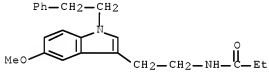
L44 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:19773 HCAPLUS Full-text
DOCUMENT NUMBER: 136:334735
TITLE: Synthesis of N1-phenethyl substituted indole derivatives as new melatoninergic agonists and antagonists
AUTHOR(S): Tsotinis, Andrew; Vlachou, Margarita; Eleutheriades, Andreas; Prinea, Effie; Ebreo, Darren; The, Muy-Teck; Sugden, David
CORPORATE SOURCE: School of Pharmacy, Department of Pharmaceutical Chemistry, University of Athens, Athens, 157 71, Greece
SOURCE: Chemical & Pharmaceutical Bulletin (2002), 50(1), 31-39
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:334735

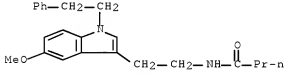
AB The potency of new indolic N1-phenethyl substituted melatoninergic ligands with and without Me groups in the α and β position of the alkanamidoethyl side chain was examined using the pigment aggregation response in a clonal line of Xenopus laevis melanophores. The non 5-OMe substituted compds. are all weak antagonists while introduction of the 5-OMe group increases both agonist and antagonist activity except in all but one case. Introduction of an α-Me group into the 5-OMe derivs. reduces the agonist potency while introduction of a β-Me group has only a small effect on either the agonist or antagonist potency. Double β-Me substitution of the 5-OMe derivs. generally increases the agonist potential and decreases the antagonist potency with one exception.

IT 416861-02-4P 416861-03-5P 416861-07-9P
416861-08-0P 416861-12-6P 416861-13-7P
416861-17-1P 416861-18-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of phenethyl substituted indole derivs. as melatoninergic agonists and antagonists)

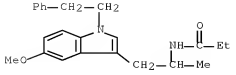
RN 416861-02-4 HCAPLUS
CN Propanamide, N-[2-[5-methoxy-1-(2-phenylethyl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 416861-03-5 HCAPLUS
CN Butanamide, N-[2-[5-methoxy-1-(2-phenylethyl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 416861-07-9 HCAPLUS
CN Propanamide, N-[2-[5-methoxy-1-(2-phenylethyl)-1H-indol-3-yl]-1-methylethyl]- (CA INDEX NAME)



RN 416861-08-0 HCAPLUS
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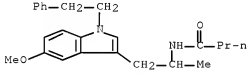
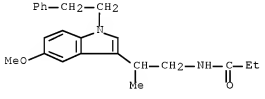
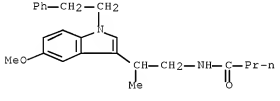


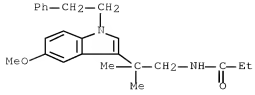
RN 416861-12-6 HCAPLUS
CN Propanamide, N-[2-[5-methoxy-1-(2-phenylethyl)-1H-indol-3-yl]propyl]- (CA INDEX NAME)



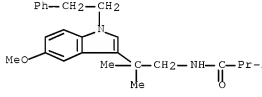
RN 416861-13-7 HCAPLUS
CN Butanamide, N-[2-[5-methoxy-1-(2-phenylethyl)-1H-indol-3-yl]propyl]- (CA INDEX NAME)



RN 416861-17-1 HCAPLUS
CN Propanamide, N-[2-[5-methoxy-1-(2-phenylethyl)-1H-indol-3-yl]-2-methylpropyl]- (CA INDEX NAME)



RN 416861-18-2 HCAPLUS
CN Butanamide, N-[2-[5-methoxy-1-(2-phenylethyl)-1H-indol-3-yl]-2-methylpropyl]- (CA INDEX NAME)



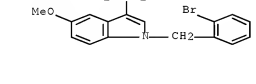
OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:185117 HCAPLUS Full-text
DOCUMENT NUMBER: 132:273842
TITLE: Mapping the Melatonin Receptor. 6. Melatonin Agonists and Antagonists Derived from 6H-Isoindolo[2,1-a]indoles, 5,6-Dihydroindolo[2,1-a]isoquinolines, and 6,7-Dihydro-5H-benzo[c]azepino[2,1-a]indoles
AUTHOR(S): Faust, Ruediger; Garratt, Peter J.; Jones, Rob; Yeh, Li-Kuan; Tsotinis, Andrew; Panoussopoulou, Maria; Calogeropoulou, Theodora; Teh, Muy-Teck; Sugden, David
CORPORATE SOURCE: Department of Chemistry, University College London, London, WC1H 0AJ, UK
SOURCE: Journal of Medicinal Chemistry (2000), 43(6), 1050-1061
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 6H-Isoindolo[2,1-a]indoles, 5,6-dihydroindolo[2,1-a]isoquinolines, and 6,7-dihydro-5H-benzo[c]azepino[2,1-a]indoles have been prepared as melatonin analogs to investigate the nature of the binding site of the melatonin receptor. The affinity of analogs was determined in a radioligand binding assay using cloned human mt1 and MT2 receptor subtypes expressed in NIH 3T3 cells. Agonist and antagonist potency was measured using the pigment aggregation response of a clonal line of Xenopus laevis melanophores. The 2-methoxyisoindolo[2,1-a]indoles showed much higher binding affinities than the parent isoindoles and whereas 2-methoxyisoindolo[2,1-a]indoles were agonists in the functional assay, its cyclopropanecarbonyl derivative and parent

isoindoles were antagonists. The 2-ethoxyisoindolo[2,1-a]indoles showed reduced binding affinities compared to their methoxy analogs, while the 5-chloro derivative showed a considerable reduction in binding affinity and potency compared to acetyl 2-methoxyisoindolo[2,1-a]indole compound The 10-methoxy-5,6-dihydroindolo[2,1-a]isoquinolines had higher binding affinities than the corresponding parent indoloisoquinolines in the human receptor subtypes, and the parent compds. were antagonists whereas the 10-methoxy derivs. were agonists in the functional assay. The N-cyclobutanecarbonyl derivs. of both the parent and 10-methoxyl series had similar binding affinities and were both antagonists with similar potencies. The 11-methoxy-6,7-5H-benzo[c]azepino[2,1-a]indoles had higher binding affinities than the corresponding parent compds. at the MT2 receptor but similar affinities at the mt1 site; all of the compds. were antagonists in the functional assay. Changing 11-methoxy for 11-ethoxy decreased the binding affinity slightly, and this was more evident at the MT2 receptor. All of the derivs. investigated had either the same or a greater affinity for the human MT2 receptor compared to the mt1 receptor (range 1:1-1:132). This suggests that the mt1 and MT2 receptor pockets differ in their ability to accommodate alkyl groups in the indole nitrogen region of the melatonin mol. Two compds. were tested in functional assays on recombinant mt1 and MT2 melatonin receptors. N-butanoyl 2-(9-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethanamine was a potent agonist with some selectivity (44-fold) for the MT2 receptor, while N-butanoyl 2-(5,6,7-trihydro-11-methoxybenzo[c]cycloheptl[2,1-a]indol-13- yl)ethanamine was an MT2-preferring antagonist. Increasing the carbon chain length between N-1 of indole and the 2-Ph group from n = 1 through n = 3 leads to a fairly regular decrease in the binding affinity, but, remarkably, when n = 3, it converts the methoxy compds. from melatonin agonists to antagonists. The Xenopus melatonin receptor thus cannot accommodate an N-n-alkyl chain attached to a 2-Ph substituent with n > 2 in the required orientation to induce or stabilize the active receptor conformation.

IT 263864-85-3P 263864-86-4P 263864-89-7P
263864-90-0P 263864-99-9P 263865-00-5P
263865-04-9P 263865-05-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and structure of melatonin agonists and antagonists derived from isoindoloindoles, indoloisoquinolines, and benzoazepinoindoles)

RN 263864-85-3 HCAPLUS
CN Propanamide, N-[2-[1-[(2-bromophenyl)methyl]-5-methoxy-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 263864-86-4 HCAPLUS
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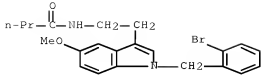
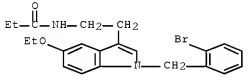
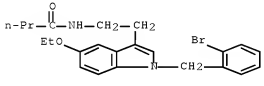


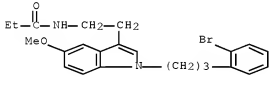
RN 263864-89-7 HCAPLUS
CN Propanamide, N-[2-[1-[(2-bromophenyl)methyl]-5-ethoxy-1H-indol-3-yl]ethyl]-
(CA INDEX NAME)



RN 263864-90-0 HCAPLUS
CN Butanamide, N-[2-[1-[(2-bromophenyl)methyl]-5-ethoxy-1H-indol-3-yl]ethyl]-
(CA INDEX NAME)



RN 263864-99-9 HCAPLUS
CN Propanamide, N-[2-[1-[3-(2-bromophenyl)propyl]-5-methoxy-1H-indol-3-
yl]ethyl]- (CA INDEX NAME)



RN 263865-00-5 HCAPLUS
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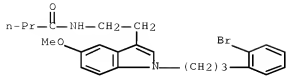
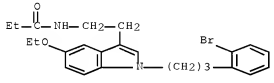
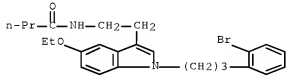
yl]ethyl]- (CA INDEX NAME)



RN 263865-04-9 HCAPLUS
CN Propanamide, N-[2-[1-[3-(2-bromophenyl)propyl]-5-ethoxy-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



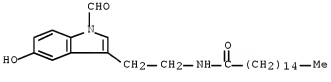
RN 263865-05-0 HCAPLUS
CN Butanamide, N-[2-[1-[3-(2-bromophenyl)propyl]-5-ethoxy-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 73 THERE ARE 73 CAPLUS RECORDS THAT CITE THIS RECORD (74 CITINGS)
REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:454201 HCAPLUS Full-text
DOCUMENT NUMBER: 129:230562
ORIGINAL REFERENCE NO.: 129:46915a,46918a
TITLE: The chemistry of indoles. 87. Syntheses of 1-hydroxytryptamines and serotonins having fatty acyl or (E)-3-phenylpropenoyl derivatives as a Nb-substituent, and a novel homologation on the 3-substituent of the 1-hydroxytryptamines upon treatment with diazomethane
AUTHOR(S): Somei, Masanori; Morikawa, Harunobu; Yamada, Koji; Yamada, Fumio
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Kanazawa University, Kanazawa, 920-0934, Japan
SOURCE: Heterocycles (1998), 48(6), 1117-1120
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:230562
AB 1-Hydroxytryptamines with (E)-3-phenyl-, (E)-3-(4-hydroxyphenyl)-, (E)-3-(4-hydroxy-3-methoxyphenyl)propenoyl, octanoyl, hexadecanoyl, and docosanoyl groups as the Nb-substituent were prepared for the first time. Prepns. of serotonins from the corresponding 1-hydroxytryptamines are also reported. A new homologation on the 3-substituent of 1-hydroxytryptamines was discovered upon treatment with diazomethane in chloroform or dichloromethane.
IT 212707-55-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fatty acyl or (E)-3-phenylpropenoyl derivs. of 1-hydroxytryptamines and serotonins and a novel diazomethane homologation on the 3-substituent of the 1-hydroxytryptamines)
RN 212707-55-6 HCAPLUS
CN Hexadecanamide, N-[2-(1-formyl-5-hydroxy-1H-indol-3-yl)ethyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1982:615988 HCAPLUS Full-text
DOCUMENT NUMBER: 97:215988
ORIGINAL REFERENCE NO.: 97:36249a,36252a
TITLE: Compound and composition for treating tumors
INVENTOR(S): Horst, Hans Joerg
PATENT ASSIGNEE(S): Fed. Rep. Ger.
SOURCE: Ger. Offen., 16 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3105850	A1	19820819	DE 1981-3105850	19810218
PRIORITY APPLN. INFO.:			DE 1981-3105850	19810218

OTHER SOURCE(S): CASREACT 97:215988; MARPAT 97:215988
GI

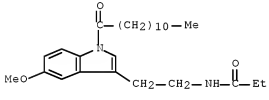
Page 42 of 44

AB Tryptamine derivs. I (R = Me, Et; R1, R2 = acyl moiety of a C9-15 carboxylic acid; R3 = H, Me; R4 = H, halo), useful in treating tumors of sex hormone-dependent organs, tissues, and(or) cells, were prepared O-Methylating 3,4-Me(O2N)C6H3OH with Me2SO4 in MeOH containing K2CO3 gave 90-95% 3,4-Me(O2N)C6H3OMe which was reduced and cyclized by catalytic hydrogenation (e.g., over Raney Ni) to give .apprx.50% 5-methoxyindole. This was cyanomethylated (successive HCHO and NaCN treatments) to give 3-(cyanomethyl)-5-methoxyindole which was reduced with BH4-, AlH3, or LiAlH4 to give 5-methoxytryptamine. This was acetylated with Ac2O to give II (R5 = H) which was acylated with Me(CH2)10COCl to give .apprx.95% diacyl derivative II [R5 = Me(CH2)10CO]. At 6 μg/mL II [R5 = Me(CH2)10CO], the prostate of a hamster gained 29.2 ± 7.3 mg, whereas when II (R5 = H) was used, the weight gain was 36.6 ± 7.5 mg, vs. 59.5 ± 11.2 for a control.

IT 83792-50-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 83792-50-1 HCAPLUS

CN Propanamide, N-[2-[5-methoxy-1-(1-oxododecyl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



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L29            19 SEA SUB=L5 SSS FUL L28
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L35           243 SEA SUB=L5 SSS FUL L34
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L37            38 SEA SUB=L35 SSS FUL L36
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L40             3 SEA ABB=ON  PLU=ON  L39 NOT L38
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L42             0 SEA ABB=ON  PLU=ON  L41 NOT (L38 OR L40)
                  D STAT QUE L42
L43             9 SEA ABB=ON  PLU=ON  L37
L44             9 SEA ABB=ON  PLU=ON  L43 NOT (L38 OR L40)
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                  D IBIB ABS HITSTR L44 1-9

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